Stark mixing of 2S muonic helium. I. Collisions with hydrogen atoms

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(Received 23 December 1987)

The transitions between the $2S$ and $2P$ states of the muonic helium atom ($\alpha\mu$ or ^{3}He-μ) in collisions with hydrogen atoms are examined using the rectilinear-trajectory coupled-equation method. The $2S$ level shift is included semiempirically and the target atom is approximated using the frozen ground-state charge density. Partial decoupling of the coupled equations is achieved, and some simple approximations for the $2S$-to-$2P$ transition probability are derived and compared with the exact solution of the coupled equations. The cross section obtained is fit by $\sigma_{2S\text{-}2P} \cong 5.5\times 10^{-3}/v^{1.8}a_0^2$ for $v \gtrsim 1$, with the velocity v in atomic units, and muon-catalyzed fusion parameters are reevaluated using this expression.

I. INTRODUCTION

The hydrogenic-atom collisional Stark mixing rate of the metastable $2S$ state into the $2P$ states is of interest for a variety of physical problems.[1-4] One such problem occurs in the theory of muon-catalyzed d-t and d-d fusion. The muon may stick to the charged fusion particle to form muonic helium ($\alpha\mu$ at 3.47 MeV in d-t fusion or ^{3}He-μ at 0.79 MeV in d-d fusion). The sticking may occur in an excited state, or the atom may be promoted there by subsequent collisions.[5] To describe the muon-catalyzed fusion kinetics, the Stark mixing rates for the metastable $2S$ state in collisions with D_2, etc., are required. Due to collisional slowing of the muonic helium ion, the mixing rates are needed for velocities below the initial $\alpha\mu$ velocity of 5.83 a.u. (the atomic unit of velocity equals αc, where α is the fine-structure constant and c is the speed of light). The present work examines this problem using the formulation of Kodosky and Leon.[4]

The Kodosky-Leon approach assumes that the hydrogenic atom (or ion) follows a straight-line trajectory relative to the target described by a screened Coulomb potential. The interaction is taken in the dipole approximation. Assuming a spin-free basis of the four $n=2$ eigenfunctions readily leads to a system of four coupled first-order differential equations. The model allows the energy of the S state to be shifted semiempirically to take into account the effect of vacuum polarization on the energy of the S states of muonic atoms. The much smaller splitting between the $2P_{1/2}$ and $2P_{3/2}$ states, which can be taken into account only if the muon spin is included in the problem,[6] is not expected to have any important consequences and is neglected in this model.

The target in most experiments is actually a hydrogen molecule rather than an atom. The results obtained in the present paper are the Stark mixing cross sections for $\alpha\mu$ in collisions with H, D, or T atoms, represented by shielded Coulomb potentials. The physics of the molecular problem is more involved and there is much to be learned by studying this simpler system first. The insight gained in the present work is useful for determining which physical ingredients need to be included in the molecular calculation.

The organization of this paper is as follows. Section II contains a discussion of the coupled-equation approach and its application to the calculation of the $2S$-$2P$ mixing cross section. In Sec. III we examine the fixed-field approximation proposed by Leon and Bethe[7] for the solution of the coupled equations. In Sec. IV we propose analytical approximations for the $2S$-$2P$ transition probability that are expected to work for the large- and small-impact-parameter regimes. The numerical results obtained from the various approaches are presented and discussed in Sec. V. Section VI discusses the application of this work to muon-catalyzed fusion.

II. THE COUPLED EQUATIONS

The Kodosky-Leon (KL) model[4] assumes that the classical straight-line trajectory approximation is valid and that the collision takes place with a constant relative velocity v at an impact parameter ρ. The basis for the mixing process is taken to be the n^2 eigenfunctions with quantum number n, situated in the rotating frame defined by the atom-target orientation vector. The S-state energy lies at ΔE_0 relative to the energy of the nonspherically symmetric states, which are taken to be degenerate. For the states considered in the present work, the separation between the $n=2$ levels and the $n=1$ or $n=3$ levels is very large compared with the $2S$-$2P$ splitting, so the $n=2$ single-manifold approximation is expected to work well.

The specific problem considered here is somewhat different from those considered by Leon and Bethe[7] (LB) and KL, so we begin by rewriting the KL equations in a slightly more general form. Including the functional dependence of the coupled equations on the nuclear charge Z and the reduced mass M_μ of the hydrogenic projectile and the screening constant β of the shielded Coulomb potential target, we obtain

$$i\dot{a}_l^m=\tfrac{3}{2}nF\left[\left[\frac{(l^2-m^2)(n^2-l^2)}{(2l+1)(2l-1)}\right]^{1/2}a_{l-1}^m+\left[\frac{[(l+1)^2-m^2][n^2-(l+1)^2]}{(2l+3)(2l+1)}\right]^{1/2}a_{l+1}^m\right]$$
$$-\tfrac{1}{2}i\dot{\theta}\left[\left[l(l+1)-m(m-1)\right]^{1/2}a_l^{m-1}-\left[l(l+1)-m(m+1)\right]^{1/2}a_l^{m+1}\right]+\delta_{l0}\delta_{m0}\Delta E_0 a_0^0\ , \tag{1}$$

where

$$F(t)=e^{-2\beta R}(1+2\beta R+2\beta^2R^2)/(ZM_\mu R^2)\ , \tag{2}$$

$$R(t)=(\rho^2+v^2t^2)^{1/2}\ , \tag{3}$$

and

$$\dot{\theta}(t)=\frac{\rho v}{\rho^2+v^2t^2}\ . \tag{4}$$

$R(t)$ denotes the distance of the atom from the target as a function of time. The zero of time t is taken at the distance of closest approach [i.e., $R(0)=\rho$] and $\theta(t)$ is the angle of the atom-target orientation vector at time t relative to that at $t=0$. For the parameter values $\beta=Z=1$ the above equations reduce to those of KL, and if in addition $\Delta E_0=0$, the equations reduce to those of LB.

With Eq. (1) specialized to $n=2$, the primary concern of the present work, it is convenient to define the vector

$$\underline{a}=\begin{bmatrix}a_0^0\\a_1^{-1}\\a_1^0\\a_1^1\end{bmatrix}\ . \tag{5}$$

Then the coupled equations are given by

$$i\dot{\underline{a}}=\underline{V}\underline{a}\ , \tag{6}$$

where

$$\underline{V}=\begin{bmatrix}\Delta E_0 & 0 & 3F & 0\\ 0 & 0 & \frac{\sqrt{2}}{2}i\dot{\theta} & 0\\ 3F & \frac{-\sqrt{2}}{2}i\dot{\theta} & 0 & \frac{\sqrt{2}}{2}i\dot{\theta}\\ 0 & 0 & \frac{-\sqrt{2}}{2}i\dot{\theta} & 0\end{bmatrix}\ . \tag{7}$$

The fact that $\underline{V}$ is Hermitian implies that the norm of $\underline{a}(t)$ remains constant as a function of time.[8] The initial conditions imposed at time t_0 must satisfy the constraint that $|\underline{a}(t_0)|=1$, because the model assumes that the population is entirely in the $n=2$ manifold. By the conservation of the norm, then $|\underline{a}(t)|=1$ for all t; therefore the model conserves probability.

The particular problem of interest for the current work is to find the vector $\underline{a}(\infty)$ given the initial condition

$$\underline{a}(-\infty)=\begin{bmatrix}1\\0\\0\\0\end{bmatrix}\ ; \tag{8}$$

i.e., prior to the collision the atom is entirely in the $2S$ state, and after the collision the components of $\underline{a}$ are desired in order to determine the probability that the atom has made a transition to one of the $2P$ states. The problem is completely determined once the parameters ρ, v, Z, β, and M_μ have been specified. However, some additional manipulations prove numerically advantageous.

Any decoupling of the system of Eqs. (6) and (7) is useful, and by introduction of the new vector $\underline{c}$ related to the components of $\underline{a}$ by

$$\underline{c}=\begin{bmatrix}c_1\\c_2\\c_3\\c_4\end{bmatrix}=\begin{bmatrix}a_0^0\\ \frac{1}{\sqrt{2}}(a_1^{-1}-a_1^1)\\ a_1^0\\ \frac{1}{\sqrt{2}}(a_1^{-1}+a_1^1)\end{bmatrix} \tag{9}$$

one obtains the new system

$$i\dot{\underline{c}}=\underline{W}\underline{c}\ , \tag{10}$$

where

$$\underline{W}=\begin{bmatrix}\Delta E_0 & 0 & 3F & 0\\ 0 & 0 & i\dot{\theta} & 0\\ 3F & -i\dot{\theta} & 0 & 0\\ 0 & 0 & 0 & 0\end{bmatrix} \tag{11}$$

and the initial condition for the problem is

$$\underline{c}(-\infty)=\begin{bmatrix}1\\0\\0\\0\end{bmatrix}\ . \tag{12}$$

Clearly the c_4 component is decoupled from the rest of the system and, in fact, is zero for all times. Thus it is only necessary to propagate the first three components of $\underline{c}$ using the upper-left block of $\underline{W}$. This block is Hermitian, so the first three components of $\underline{c}$ conserve probability. Finally, the mixing probability of interest $P_{2S\text{-}2P}^{\mathrm{FSM}}$ is defined by

$$P_{2S\text{-}2P}^{\mathrm{FSM}}=|c_2(\infty)|^2+|c_3(\infty)|^2\ , \tag{13}$$

where FSM designates the "full Stark model" in order to distinguish this result from the various approximations for the transition probability discussed later. Equations (2)–(4) and (10)–(13) constitute the problem in the final form.

All that remain to be considered are the computational details of the calculation. The propagation of Eq. (10)

can be accomplished by any one of several numerical approaches. The technique used in the present work is the Adams-Bashforth-Moulton predictor-corrector method. Most of the available codes are designed for the propagation of real systems; however, Eq. (10) can be easily rewritten in real and imaginary component form, yielding a system of six real coupled equations. An integration distance of a few screening lengths is adequate for the calculation, and the system appears to be well behaved for the values of parameters examined here.

Once the mixing probability is known as a function of impact parameter, the Stark mixing cross section is easily obtained by

$$\sigma_{2S\text{-}2P}=2\pi\int_0^\infty d\rho\,\rho P_{2S\text{-}2P}\ . \tag{14}$$

This integral is performed by numerical quadrature.

III. THE LEON-BETHE FIXED-FIELD MODEL

The model described in Sec. II contains most of the important physical interactions, and the resulting numerical solutions are expected to yield accurate results for the mixing probabilities. Nevertheless, it is of interest to examine whether simple approximations can yield reasonable results with less effort. For the present work, these further simplifications are primarily a matter of convenience since the numerical propagation of the three coupled equations is not especially difficult. For large n, the question becomes more critical because the number of coupled equations grows as n^2, and the system can quickly become so large that direct solution of the coupled equations is either too expensive or numerically difficult. This was the case for the mesic atom cascade process investigated by LB, who were led to consider solutions of the system for levels as high as $n=23$; the accurate propagation of the associated 1058-real-component solution vector would appear to be rather difficult, even by today's computational standards.

For problems where the energy shift ΔE_0 can be neglected, an approximation known as the fixed-field model is of interest. LB proposed that, for transitions in and out of the S states, the neglect of the angular coupling terms present in Eq. (1) should provide a coupled system whose solutions are in reasonable agreement with those of the original system. They term the approximation the fixed-field model (FFM) and apply it to *slow* collisions of mesic hydrogen atoms with normal hydrogen atoms. Such an approach certainly achieves the goal of simplifying the coupled system, because, in the Stark representation, the equations completely decouple and can be solved in analytical form. In addition, LB make a further approximation that leads to an extremely simple semianalytical method for obtaining the Stark mixing cross section.

In the present paper the cross section is obtained without recourse to such approximations. Nevertheless, it is of interest to compare the exact numerical solution of the full Stark model with the fixed-field model solution and the LB approximation to the fixed-field cross section. This section contains a brief summary of the LB results for the fixed-field model, written out in a somewhat more convenient form for purposes of computation.

The basic fixed-field model result obtained by LB is that, for the manifold n, if the atom has unit probability of being in the S state before the collision, then the probability that it is still in the S state after the collision is

$$P_{nS\text{-}nS}^{\mathrm{FFM}}=\frac{1}{n^2}\left|\sum_{j=0}^{n-1}e^{-i\Phi(n;j)}\right|^2 , \tag{15}$$

where the "Stark phase" $\Phi(n;j)$ is given by

$$\Phi(n;j)=\frac{3\pi n(2j-n+1)}{2Zv\rho M_\mu}\zeta(\beta\rho)\ , \tag{16}$$

and the function ζ is defined by the integral

$$\zeta(x)=\frac{1}{\pi}\int_{-\pi/2}^{\pi/2}d\theta\,e^{-2x\sec\theta}(1+2x\sec\theta+2x^2\sec^2\theta)\ . \tag{17}$$

Equation (16) has been generalized to include the functional dependence on Z and β, which are both unity in the LB problem. The fixed-field model results are given by LB essentially in the above form, and the integral of Eq. (17) is to be performed numerically.

For purposes of calculation we provide expressions that are somewhat easier to use than Eqs. (15)–(17). Inserting Eq. (16) into Eq. (15) and performing the summation one obtains

$$P_{nS\text{-}nS}^{\mathrm{FFM}}=\frac{1}{n^2}\left[1-2\cos\left[\frac{(n-1)\Delta\Phi(n)}{4}\right]\times\sin\left[\frac{(n+1)\Delta\Phi(n)}{4}\right]\times\mathrm{cosec}\left[\frac{\Delta\Phi(n)}{2}\right]\right]^2 \tag{18}$$

for n odd, and

$$P_{nS\text{-}nS}^{\mathrm{FFM}}=\frac{1}{n^2}\left[\sin\left[\frac{n\Delta\Phi(n)}{2}\right]\mathrm{cosec}\left[\frac{\Delta\Phi(n)}{2}\right]\right]^2 \tag{19}$$

for n even, where

$$\Delta\Phi(n)=\frac{3\pi n}{Zv\rho M_\mu}\zeta(\beta\rho)\ . \tag{20}$$

Although Eq. (17) can be integrated numerically without difficulty, an analytical expression is more convenient. The integral of Eq. (17) can, in fact, be performed analytically and one finds[9]

$$\zeta(x)=1-2x[L_0(2x)K_1(2x)+L_1(2x)K_0(2x)]+\frac{4x^2}{\pi}K_1(2x)\ , \tag{21}$$

where K_0 and K_1 are modified Bessel functions and L_0 and L_1 are modified Struve functions. Expansions for all these functions are provided in Ref. 10. Although subroutines are available for K_0 and K_1, Struve-function subroutines appear to be quite scarce. Thus we provide a simple analytical expression below for $\zeta(x)$ that seems to be adequate for most purposes. We break the domain of

definition of the approximation $\tilde{\zeta}(x)$ to $\zeta(x)$ into three ranges:

$$\tilde{\zeta}(x)=1-\frac{2}{\pi}x+\frac{4}{3\pi}x^3\ln x+ax^3+bx^4 , \tag{22}$$

where $a=0.3550$ and $b=-0.3338$ for $0<x<1$,

$$\tilde{\zeta}(x)=(0.890+1.665x+0.289x^2)e^{-2x} \tag{23}$$

for $1<x<2$, and,

$$\tilde{\zeta}(x)=\frac{2}{\sqrt{\pi}}x^{3/2}e^{-2x}\left[1+\frac{a}{x}+\frac{b}{x^2}\right] , \tag{24}$$

where $a=1.190$ and $b=0.360$ for $x>2$. The above approximation $\tilde{\zeta}(x)$ lies within 0.1% of the exact function $\zeta(x)$ over the entire domain $(0,\infty)$. This analytical interpolative approximation can be easily extended to include more terms in the expansions if greater accuracy is required.

In the current work, we limit our attention to the special case of $n=2$. Then Eq. (19) reduces to

$$P_{2S\text{-}2S}^{\mathrm{FFM}}=\cos^2\left[\frac{\Delta\Phi(2)}{2}\right] , \tag{25}$$

where

$$\Delta\Phi(2)=\frac{6\pi}{Zv\rho M_\mu}\zeta(\beta\rho) . \tag{26}$$

Values of the function ζ in Eq. (26) are easily obtained through use of the approximation $\tilde{\zeta}$ defined in Eqs. (22)–(24). The mixing cross section is then obtained in a fashion similar to that of Eq. (14) using

$$\sigma_{2S\text{-}2P}^{\mathrm{FFM}}=2\pi\int_0^\infty d\rho\,\rho(1-P_{2S\text{-}2S}^{\mathrm{FFM}}) . \tag{27}$$

The integral in Eq. (27) is readily performed by numerical quadrature. The fixed-field approximation is compared with other approximate formulations and with direct solution of the coupled equations in Sec. V.

In addition to the fixed-field approximation, LB consider a further approximation to reduce the effort required to evaluate integrals of the type appearing in Eq. (27). A semianalytical approximation is derived that appears to be applicable only to collisions in large-n states for which the bulk of the cross section arises over impact parameters where the interaction is strong. The method relies on the sharp cutoff of the transition probability due to screening to eliminate appreciable contributions from the perturbative region, a reasonable approximation for slow collisions. This approximation does not appear to be useful for the present high-velocity collisions because here the majority of the cross section arises over impact parameters where the interaction is weak. The present collision satisfies neither the large-n nor the low-velocity criterion, and we merely note that application of the technique to this problem leads to substantial errors (though, as it turns out, the error is opposite that of the fixed-field approximation itself, so some fortuitous cancellation occurs). Thus it is necessary to perform the integrals directly by numerical quadrature.

IV. APPROXIMATIONS FOR THE 2S-2P TRANSITION PROBABILITY

Section III contained a discussion of the LB fixed-field model, which leads to extremely simple expressions (even for large n) for the transition probability in and out of the S state. In this section we limit our attention to just the $n=2$ manifold, and examine the possibility of obtaining more sophisticated approximations for the 2S-2P transition probability. The small number of coupled equations involved means a more careful examination is possible. The derivation of the approximation is facilitated by considering the large- and small-impact-parameter regimes separately.

The large-impact-parameter regime, where the effect of the collision on the system is weak, is the most straightforward case to consider. The choice of approximation for this case is clearly a time-dependent perturbative approach. The treatment used to obtain the first-order perturbation result for the transition probability will be described fully elsewhere,[11] so here we only list the final results. Upon performing the analysis one finds that, in the first-order time-dependent perturbation-theory (PT) approximation, the transition probability out of the 2S state is given by

$$P_{2S\text{-}2P}^{\mathrm{PT}}(\rho)=[I_+(\rho)]^2+[I_-(\rho)]^2 , \tag{28}$$

with

$$I_\pm(\rho)=\frac{3\sqrt{2}}{Zv^2M_\mu}\int_0^\infty dt\,s^{-2}(1+2\lambda S+2\lambda^2s^2)e^{-2\lambda s}\times\cos\left[\omega t\pm\arctan\left[\frac{t}{\tau}\right]\right] , \tag{29}$$

where we have introduced

$$s(t)=(t^2+\tau^2)^{1/2} ,$$

$$\omega=\Delta E_0 ,$$

$$\tau=\rho/v ,$$

and

$$\lambda=\beta v .$$

The integral of Eq. (29) appears to be too complicated to evaluate in closed form; nevertheless, the real, one-dimensional integral is computationally much easier to deal with than the propagation of the coupled system of Eq. (10).

For $\omega=0$, however, the integral of Eq. (29) can be evaluated analytically. For this special case, $I_+(\rho)$ and $I_-(\rho)$ have the same value, designated here by $I_0(\rho)$, and after a change of the integration variable the integral can be written in the form

$$I_0(\rho)=\frac{3\sqrt{2}}{Zv\rho M_\mu}\int_1^\infty dy\frac{e^{-\gamma y}[1+2\gamma y+2\gamma^2y^2]}{y^2(y^2-1)^{1/2}} , \tag{30}$$

where we have introduced $\gamma=\beta\rho$. Using Eq. 8.432.3 of Ref. 12, along with "Feynman's trick" of generating new integrals by integrating with respect to a parameter under the integral sign,[13,14] one easily obtains

$$\int_1^\infty dy\frac{e^{-2\gamma y}}{y^j(y^2-1)^{1/2}}=\mathrm{Ki}_j(2\gamma) \tag{31}$$

for all integer values of j, where Ki_j is the modified Bessel integral function as defined in Ref. 10. This result does not appear to be contained in the standard reference[12] under any guise. Using the expressions for the Ki_j obtained from Ref. 10, one obtains the final result

$$I_0(\rho)=\frac{6\sqrt{2}\beta}{Zv M_\mu}[\beta\rho K_0(2\beta\rho)+K_1(2\beta\rho)] , \tag{32}$$

where K_0 and K_1 are modified Bessel functions, and a fortuitous cancellation has eliminated a rather unpleasant expression involving modified Struve functions.

Inserting the result from Eq. (32) into the equation corresponding to Eq. (28), one finds that, in the degenerate-level first-order time-dependent perturbation theory (DPT) approximation, the transition probability out of the $2S$ state is given by

$$P^{\mathrm{DPT}}_{2S\text{-}2P}(\rho)=\left[\frac{12\beta}{Zv M_\mu}\right]^2[\beta\rho K_0(2\beta\rho)+K_1(2\beta\rho)]^2 . \tag{33}$$

The transition probability in this approximation violates conservation of probability for small enough ρ, because $P^{\mathrm{DPT}}_{2S\text{-}2P}(\rho)$ diverges as ρ^{-2} for small ρ. However, the expression is expected to be valid for large ρ in situations for which the level splitting can be neglected.

The effect of a nonzero splitting ω is to provide a cutoff for the transition probability at large impact parameters. As will be seen below, the cross-section integral of the degenerate Coulomb model diverges logarithmically with the upper limit. A nonzero splitting suppresses this divergence.[11] In the present model the assumption of a *shielded* Coulomb potential provides a cutoff on the order of a screening length, even if the splitting ω is taken to be zero. For the splitting to have any substantial effect, ω must be large enough that the "characteristic length" of the cutoff associated with ω is less than the screening length β^{-1}. Thus, for very small ω, the splitting may have very little effect on the probability at *any* impact parameter for the shielded Coulomb model. For such situations, Eq. (33) should serve as an accurate approximation at large impact parameters.

Now consider the small-impact-parameter regime. In keeping with the previous comments about the role of the splitting, we here set $\omega=0$ at the onset. Clearly, in this region perturbation theory cannot be used and what is needed is some type of analytically soluble coupled-equation approach. An appropriate choice for this would appear to be the degenerate Coulomb model (DCM), first examined by Chibisov.[3] For small enough impact parameters (and high velocities), it seems reasonable that most of the mixing occurs near enough to the nucleus that shielding can also be neglected.

Chibisov's degenerate Coulomb result for the transition probability out of the $2S$ state is given by

$$P^{\mathrm{DCM}}_{2S\text{-}2P}(\rho)=\frac{q}{(1+q)^2}\left[4\sin^2\left[\frac{\pi}{2}\sqrt{1+q}\right]+q\sin^2\left[\pi\sqrt{1+q}\right]\right] , \tag{34}$$

with

$$q=\frac{9}{Z^2v^2\rho^2M_\mu^2} ,$$

where we have introduced the functional dependence of q upon Z and M_μ, both taken to be unity in Chibisov's derivation. It is easily checked that $P^{\mathrm{DCM}}_{2S\text{-}2P}(\rho)$ falls off as ρ^{-2} for large impact parameters. Thus when Eq. (34) is inserted into Eq. (14) to obtain the cross section, the resulting expression diverges logarithmically with the upper limit. The transition probability of Eq. (34) can be demonstrated to be less than or equal to unity for all real positive ρ, so the degenerate Coulomb model conserves probability. For small ρ, $P^{\mathrm{DCM}}_{2S\text{-}2P}(\rho)$ has an oscillatory character with the oscillations increasingly rapid as ρ goes to zero.

We have obtained expressions for the $2S$-$2P$ transition probability in this section that we expect to be valid for large and small impact parameters. The analytical expressions given by Eqs. (33) and (34) both assume degenerate levels, while the perturbation result for large impact parameters given by Eqs. (28) and (29) includes the splitting; however, the integral must be evaluated numerically. In Sec. V we evaluate the approximate expressions discussed in this section and compare the results with those obtained from the full Stark and fixed-field models.

V. NUMERICAL RESULTS

In this section we present results obtained using the formulations described in Secs. II–IV. All the necessary calculations are straightforward once the parameters describing the collision have been specified. For the problem at hand we have $Z=2$ and $M_\mu=201.069m_e$, where m_e is the mass of the electron. For the energy splitting of $\alpha\mu$ it is necessary to neglect the energy difference between the $2P$ states (due to the absence of spin in the model); thus, we take the average, $\Delta E_0=E(2S_{1/2})-\frac{1}{3}[E(2P_{1/2})+2E(2P_{3/2})]=-0.0543$ in electronic atomic units.[15] In addition, we shall also consider the complete neglect of the energy splitting (i.e., $\Delta E_0=0$). The remaining parameters, ρ, v, and β, are of interest for a range of values to be specified when needed.

For the first calculation we consider the case of the collision parameters $\beta=1$ and $v=5.83$ a.u. These values correspond to the problem of primary interest. This velocity is that of the $\alpha\mu$ fragment immediately after the decay of the compound nucleus, and $\beta=1$ is the shielding constant of the hydrogen atom in the $1S$ state. Table I contains the Stark mixing transition probability $P_{2S\text{-}2P}$, as a function of impact parameter, obtained from the full Stark model, the fixed-field model, and the large- and small-impact-parameter approximations discussed in Sec. IV.

The results of Table I indicate that for impact parameters less than $5.0\times10^{-2}a_0$, $P^{\mathrm{DCM}}_{2S\text{-}2P}(\rho)$ serves as a good approximation to $P^{\mathrm{FSM}}_{2S\text{-}2P}(\rho)$, while for impact parameters above $5.0\times10^{-2}a_0$, $P^{\mathrm{DPT}}_{2S\text{-}2P}(\rho)$ accurately represents $P^{\mathrm{FSM}}_{2S\text{-}2P}(\rho)$. The analytical approximations used in this manner are thus capable of providing the transition prob-

TABLE I. Transition probabilities at $v=5.83$ a.u. calculated in different approximations. FSM is the full Stark model, FFM is the fixed-field model, DCM is the degenerate Coulomb model, and DPT is the degenerate-level first-order time-dependent perturbation theory for the full Stark model.

ρ (units of a_0)	$P^{\mathrm{FSM}}_{2S\text{-}2P}$	$P^{\mathrm{FFM}}_{2S\text{-}2P}$	$P^{\mathrm{DCM}}_{2S\text{-}2P}$	$P^{\mathrm{DPT}}_{2S\text{-}2P}$
1.0×10^{-4}	2.67×10^{-1}	3.60×10^{-1}	2.65×10^{-1}	$6.55\times10^{+2}$
2.0×10^{-4}	9.90×10^{-1}	8.99×10^{-1}	9.90×10^{-1}	$1.64\times10^{+2}$
5.0×10^{-4}	7.75×10^{-1}	9.67×10^{-1}	7.73×10^{-1}	$2.62\times10^{+1}$
1.0×10^{-3}	6.24×10^{-1}	5.90×10^{-1}	6.22×10^{-1}	$6.55\times10^{+0}$
2.0×10^{-3}	7.82×10^{-1}	8.21×10^{-1}	7.81×10^{-1}	$1.64\times10^{+0}$
5.0×10^{-3}	2.30×10^{-1}	5.16×10^{-1}	2.30×10^{-1}	2.62×10^{-1}
1.0×10^{-2}	6.34×10^{-2}	1.51×10^{-1}	6.34×10^{-2}	6.55×10^{-2}
2.0×10^{-2}	1.62×10^{-2}	3.89×10^{-2}	1.62×10^{-2}	1.64×10^{-2}
5.0×10^{-2}	2.60×10^{-3}	6.05×10^{-3}	2.62×10^{-3}	2.61×10^{-3}
1.0×10^{-1}	6.42×10^{-4}	1.41×10^{-3}	6.55×10^{-4}	6.42×10^{-4}
2.0×10^{-1}	1.52×10^{-4}	3.05×10^{-4}	1.64×10^{-4}	1.52×10^{-4}
5.0×10^{-1}	1.73×10^{-5}	2.89×10^{-5}	2.62×10^{-5}	1.73×10^{-5}
$1.0\times10^{+0}$	1.69×10^{-6}	2.39×10^{-6}	6.55×10^{-6}	1.69×10^{-6}
$2.0\times10^{+0}$	3.17×10^{-8}	3.92×10^{-8}	1.64×10^{-6}	3.17×10^{-8}

ability to an accuracy within 1% over the entire domain of physical interest. In the regions where these approximations individually break down, the ρ^{-2} behavior can be seen from Table I for $P^{\mathrm{DPT}}_{2S\text{-}2P}(\rho)$ at small ρ and for $P^{\mathrm{DCM}}_{2S\text{-}2P}(\rho)$ at large ρ.

Full Stark model calculations were also performed with $\Delta E_0=0$; no difference in the transition probability was detected to the number of digits reported. Therefore the vacuum polarization shift of the $2S$ level does not play a significant role in the Stark mixing dynamics for this particular collision.

The fixed-field results, while having the correct qualitative behavior, do not appear to be especially useful here if quantitative accuracy is required. For this particular physical problem (at much higher velocities than the LB problem) the rotation of the frame has too much of an effect on the physics for the neglect of the angular coupling to be a good approximation over the range of impact parameters of interest (by the "range of interest" we mean the range that contributes substantially to the integrated cross section). The results of Table I indicate that the fixed-field approximation overestimates the transition probability at medium impact parameters by about a factor of 2, while at large impact parameters the discrepancy is not as great.

Figure 1 contains plots of $P^{\mathrm{FSM}}_{2S\text{-}2P}(\rho)$, $P^{\mathrm{DPT}}_{2S\text{-}2P}(\rho)$, $P^{\mathrm{DCM}}_{2S\text{-}2P}(\rho)$, and $P^{\mathrm{FFM}}_{2S\text{-}2P}(\rho)$, for impact parameters over the range from $10^{-3}a_0$ to $1.0a_0$. The dotted, short-dashed, and long-dashed lines represent the FFM, DPT, and DCM solutions, respectively. The solid line signifies the FSM solution. The DPT and FSM solutions appear to be coincident for impact parameters greater than $10^{-2}a_0$. Near $\rho=1.0a_0$ the DCM solution is clearly failing, while for ρ less than $2.5\times10^{-3}a_0$ the DPT solution exceeds unity (thus violating conservation of probability). For impact parameters greater than $2.0\times10^{-3}a_0$, the values of $P^{\mathrm{FFM}}_{2S\text{-}2P}(\rho)$ are significantly larger than those of $P^{\mathrm{FSM}}_{2S\text{-}2P}(\rho)$, as indicated in Table I. Finally, note that when the cross section is computed using Eq. (14), the contributions from the range pictured in Fig. 1 are found to constitute the vast majority of the total.

For small impact parameters the behavior of the transition probability is too intricate for the few values listed in Table I over this range to be especially descriptive. The highly oscillatory behavior for this region is clearly visible in Fig. 2. Figure 2 contains plots of $P^{\mathrm{FSM}}_{2S\text{-}2P}(\rho)$, $P^{\mathrm{DPT}}_{2S\text{-}2P}(\rho)$, $P^{\mathrm{DCM}}_{2S\text{-}2P}(\rho)$, and $P^{\mathrm{FFM}}_{2S\text{-}2P}(\rho)$, for impact parameters over the range from $10^{-4}a_0$ to $10^{-2}a_0$. Over this range, the FSM and DCM solutions are coincident, and the DPT solution exceeds unity (and is therefore off the graph) for impact parameters less than $2.5\times10^{-3}a_0$.

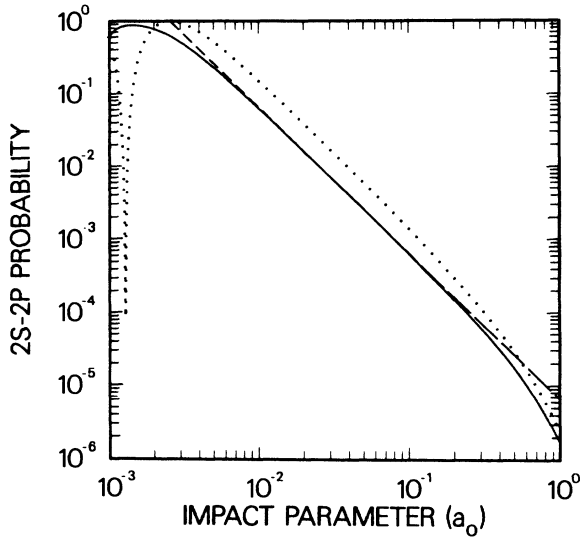

FIG. 1. Transition probability for $\alpha\mu(2S)+\mathrm{D}\rightarrow\alpha\mu(2P)+\mathrm{D}$ at velocity 5.83 a.u. in the impact parameter range $0.001a_0$ to $1.0a_0$. The full Stark model (solid curve) is compared with the fixed-field model (dotted curve), the degenerate Coulomb model (long-dashed curve), and degenerate-level first-order time-dependent perturbation theory (short-dashed curve).

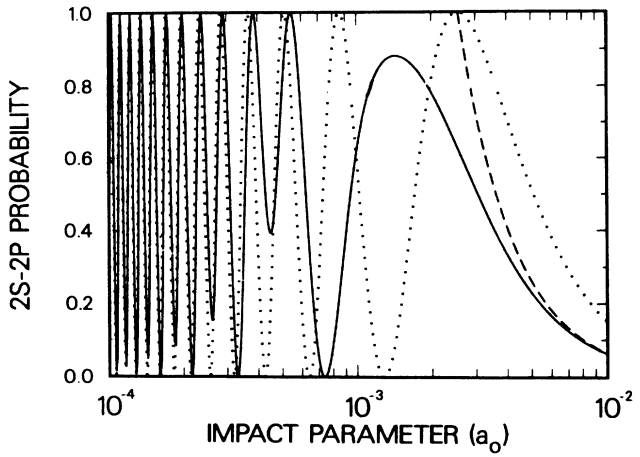

FIG. 2. Transition probability for $\alpha\mu(2S)+D\rightarrow\alpha\mu(2P)+D$ at velocity 5.83 a.u. in the impact parameter range $10^{-4}a_0$ to $10^{-2}a_0$. The curves are designated as in Fig. 1.

Thus *together* the DCM and FFM solutions cover the complete range of impact parameters.

Within $10^{-3}a_0$, both the DCM and FFM solutions exhibit an oscillatory behavior, with the oscillations increasingly rapid as ρ goes to zero. The FFM solution is simpler and shall be examined first. The probability in this case is equal to $\sin^2[\frac{1}{2}\Delta\Phi(2)]$, with $\Delta\Phi(2)$ given in Eq. (26). The extrema occur at values of ρ satisfying $\rho=6\zeta(\beta\rho)/(kZv M_\mu)$ for integer values of k; for odd k a maximum of unity is attained, while for even k a minimum of zero is attained. In the limit as ρ goes to zero, $\zeta(\beta\rho)$ approaches unity; thus the extrema occur at $\rho=6/(kZv M_\mu)$ for asymptotically small ρ.

The behavior of the DCM solution is somewhat more complicated but can be explained with the help of Eq. (34). Clearly, a minimum of zero is attained for the DCM solution at values of impact parameter for which $(1+q)^{1/2}=k$, for even integer values of k. It can also be shown, by use of elementary trigonometry, that $P^{\rm DCM}_{2S\text{-}2P}(\rho)$ attains a maximum of unity at values of ρ for which $\sin^2[\frac{1}{2}\pi(1+q)^{1/2}]=(1+q)/2q$; this transcendental equation has a denumerably infinite number of solutions. The only remaining features that need to be explained are the minima that fail to attain zero. These correspond roughly to values of ρ for which $(1+q)^{1/2}=k$ at odd integers k, where the $q\sin^2[\pi(1+q)^{1/2}]$ term of Eq. (34) is zero but the $4\sin^2[\frac{1}{2}\pi(1+q)^{1/2}]$ term is equal to 4. As q increases (i.e., as ρ decreases), the effect of the nonzero term becomes diluted; consequently, the nonzero minima do asymptotically approach zero as ρ goes to zero, as shown in Fig. 2. Further examination of the equations indicates that the DCM and FFM solutions asymptotically approach one another as ρ goes to zero. This can also be seen by inspection of Fig. 2. Thus LB's claim that the FFM solutions are satisfactory for small impact parameters is indeed true here; however, for the present problem, the range over which the FFM solution is a valid approximation to the FSM solution does not contribute very substantially to the cross section.

In Table II we examine the evaluation of the integral occurring in Eq. (14), required for the cross section. It is informative to break the $(0,\infty)$ integration range into the intervals (0,0.005), (0.005,0.5), and $(0.5,\infty)$ and to compare the contributions from these intervals separately. For Table II we define the integral

$$I(\rho_1,\rho_2)=\int_{\rho_1}^{\rho_2}d\rho\,\rho P_{2S\text{-}2P}(\rho)\ . \tag{35}$$

First consider the integral over the interval (0,0.005). The contribution from the full Stark model is $5.74\times10^{-6}a_0^2$, while the contribution from the degenerate Coulomb model is almost the same, $5.73\times10^{-6}a_0^2$, as expected from the near coincidence of the FSM and DCM solutions over this region. The contribution from the fixed-field model is $8.89\times10^{-6}a_0^2$, about 50% too high. Conservation of probability can be used to determine that the upper bound on the integral over this region is equal to $1.25\times10^{-5}a_0^2$, and from the oscillatory nature of the functions it is reasonable to estimate the integrals by introducing a factor of $\frac{1}{2}$, thus obtaining $6.25\times10^{-6}a_0^2$. All the integrals are in rough agreement with this result. Finally, the DPT solution is seen to yield a divergent contribution over this interval, but of course perturbation theory is not expected to be applicable in the region of strong interactions.

Now consider the large-impact-parameter interval $(0.5,\infty)$. As seen from Table I, the transition probability over this region is quite small and perturbation theory works extremely well. Upon performing the integrals one finds that the FSM and DPT contributions are both equal to $2.63\times10^{-3}a_0^2$. The FFM contribution is found to be $3.99\times10^{-6}a_0^2$, about 50% too high. The DCM contribution diverges, as mentioned previously, due to the long-range nature of the Coulomb interaction.

Next consider the intermediate interval (0.005,0.5). In both the full Stark and fixed-field models, the bulk of the cross section arises from contributions over this interval. The FSM contribution is found to be $2.84\times10^{-5}a_0^2$, while the FFM contribution is $6.32\times10^{-5}a_0^2$, more than

TABLE II. Integral [Eq. (35); the contribution to the cross section is given by $2\pi I(\rho_1,\rho_2)$; i.e., $\sigma=2\pi I(0,\infty)$] $I(\rho_1,\rho_2)$ at $v=5.83$ a.u. in different approximations for specified ranges of impact parameter.

(ρ_1,ρ_2)	$I^{\rm FSM}$	$I^{\rm FFM}$	$I^{\rm DCM}$	$I^{\rm DPT}$
(0,0.005)	5.74×10^{-6}	8.89×10^{-6}	5.73×10^{-6}	∞
(0.005,0.5)	2.84×10^{-5}	6.32×10^{-5}	2.97×10^{-5}	2.88×10^{-5}
$(0.5,\infty)$	2.63×10^{-6}	3.99×10^{-6}	∞	2.63×10^{-6}
$(0,\infty)$	3.68×10^{-5}	7.61×10^{-5}	∞	∞

two times too large. Over this region both the DCM and DPT contributions are in fairly good agreement with the FSM result, equal to $2.97\times10^{-5}a_0^2$ and $2.88\times10^{-5}a_0^2$, respectively.

Finally consider the entire interval $(0,\infty)$. The cross section is obtained from the integral $I(0,\infty)$ by multiplying by 2π. For the full Stark model, we obtain $\sigma_{2S\text{-}2P}^{\mathrm{FSM}}=2.31\times10^{-4}a_0^2$; for the fixed-field model $\sigma_{2S\text{-}2P}^{\mathrm{FFM}}=4.78\times10^{-4}a_0^2$, about two times too large. The DCM and DPT cross sections are of course divergent.

We find that the accurate (FSM) integrated cross for $\alpha\mu(2S)+D$ as a function of velocity can be adequately fit by a simple power law

$$\sigma_{2S\text{-}2P}\cong\frac{5.5\times10^{-3}}{v^{1.8}}a_0^2 \ . \tag{36}$$

In conclusion, we comment on the effects of the approximations remaining in the present calculations. The first question concerns the effect of deflections on the cross section. Deflections have been shown to be important in ionizing collisions of $\alpha\mu$ with H at $v\lesssim2$ a.u.[16] However, Stark transitions occur in collisions having considerably larger impact parameters, and the straight-line trajectory approximation consequently can be expected to still be a good approximation at least to velocities as small as 1 a.u.

A more serious problem may be the breakdown of the dipole approximation. Upon examining the characteristic lengths associated with the $\alpha\mu$ atom $n=2$ wave functions, one finds that the dipole approximation is reasonable *outside* the (0,0.005) interval but not well justified *within* the interval. However, the transition probability in this inner interval is saturated (i.e., oscillating between zero and unity) under the dipole approximation to the interaction and is probably also saturated under the more realistic Coulomb interaction. Therefore one expects that $I(0,0.005)\cong6.25\times10^6a_0^2$ for either of the two interactions by taking half the upper bound, as discussed earlier. This interval does not contribute very substantially to the cross section so the problems associated with the breakdown of the dipole approximation here are not especially serious. The breakdown of the dipole approximation on the low end of the (0.005,0.5) interval may be somewhat of a problem also, but we do not expect the total loss in accuracy to exceed 20%.

The present calculations neglect transitions out of the $n=2$ manifold. The error resulting from this approximation can be expected to be no greater than the ratio of the cross section for n-changing, charge-transfer, and ionizing collisions of $\alpha\mu(2S)$, which have been previously calculated,[17] to that for Stark transitions. This ratio is as large as 0.3 (at $v\cong4$ a.u.). However, the Stark transitions come mostly from larger impact parameters, so the actual error incurred is probably considerably smaller.

Next we examine the sensitivity of the cross section to variations in the shielding. The physical problem of main interest, of course, is the Stark mixing of $\alpha\mu$ due to collisions with D_2. Up to this point we have considered the problem of Stark mixing of $\alpha\mu$ due to collisions with an atomic screened Coulomb potential. The screening of the nuclei in the D_2 molecule will be somewhat different for the molecule than for two noninteracting atoms. However, if the cross section is not especially sensitive to variations in the shielding, then we can hope to model the molecule with the compound atom model. We arbitrarily modify the shielding by varying the shielding constant β. Calculations were performed with $\beta=0.9$ and 1.1, with the remaining parameters the same as used for the previous calculations. For $\beta=0.9$, the cross section was found to increase by 1.6%, while for $\beta=1.1$ the cross section was found to decrease by 1.6%. This behavior indicates that the distortion of the screening cloud due to molecular interactions is not likely to have any substantial effect on the cross section, so the compound $1S$-atom model appears to be well justified.

However, even neglecting the sensitivity of the Stark mixing to the distortion of the screening, there still remains the question of whether simple superposition of the cross sections can be used to obtain the total cross section for the compound atom model. Looking at Table II one finds that most of the contribution to the cross section comes from impact parameters between $0.005a_0$ and $0.5a_0$, a regime where perturbation theory works fairly well. For trajectories far enough away from both of the nuclei that perturbation theory is valid, there is certainly a superposition principle at work; however, it is for superposition of the *amplitudes,* not the probabilities. Thus for trajectories parallel to the internuclear axis, perturbation theory leads to a transition probability for the compound atom model that is four times that obtained for the single atom collision (at the same impact parameter). For trajectories passing very close to both nuclei, the bound on the transition probability would mean that passing near the second nucleus leads to no net gain in the cross section since the transition probability is already saturated. Cases where the trajectory passes through the neighborhood of only one of the atoms behave more simply and there are no significant molecular effects in the transition probabilities for such trajectories. A rigorous calculation of the interference effects, which explicitly takes into account the two-centered nature of the electrostatic potential, is given in the following paper.[18]

VI. EFFECT ON MUON-CATALYZED FUSION KINETICS

It has been recently shown to be necessary to separate the $2S$ and $2P$ populations of muonic helium ($\alpha\mu$ or ^{3}He-μ) for an accurate treatment of the kinetics in muon-catalyzed fusion.[5] Earlier treatments had either assumed the two levels to be populated statistically, or in some other steady-state ratio, at all times. The observed sticking fraction (including stripping) and especially x-ray production depend significantly on the Stark mixing rate. The sensitivity was shown to be greatest if the true mixing rate turned out to be *slower* than that used. In fact, as shown in Fig. 3, the present calculation gives a Stark mixing rate about a factor of 2 *faster* than that previously used and hence does not greatly alter previously accepted theoretical values of the muon-catalyzed fusion parameters.

The calculations of muonic helium kinetics in muon-

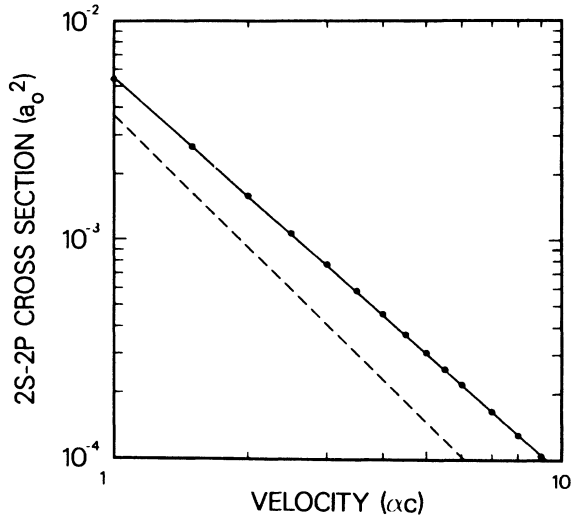

FIG. 3. Cross sections for $\alpha\mu(2S)+D\rightarrow\alpha\mu(2P)+D$ as a function of collision velocity. The data points are calculated with the full Stark model and fit (solid line) by Eq. (36). The dashed line shows the values used in Ref. 5.

catalyzed *d-t* and *d-d* fusion have been repeated using our more accurate Stark mixing rate. Because the cross section has been shown to be quite insensitive to the $2S$-$2P$ energy splitting and straight-line trajectories are a good approximation, the same Stark mixing rate can be used for ^{3}He-μ as for $\alpha\mu$. The results for muon stripping and $K\alpha$ x-ray production are given in Table III and compared with the earlier results obtained using a smaller mixing rate and with those assuming an infinite mixing rate. All other rates in these calculations are identical so the differences derive from the Stark rates. The present results turn out to be about one-third away from those obtained with the previous mixing rate toward those assuming statistical mixing. These changes do not help resolve the small remaining discrepancies with the experimental values and strongly suggest that their explanation must lie elsewhere.

TABLE III. Stripping probability R and $K\alpha$ x-ray production *per sticking* in muon-catalyzed *d-t* and *d-d* fusion obtained using different $2S$-$2P$ Stark mixing rates.

	R		$N_{K\alpha}$	
	$\phi=1.2$	$\phi=0.05$	$\phi=1.2$	$\phi=0.05$
Muon-catalyzed *d-t* fusion				
Present[a]	0.351	0.290	0.301	0.360
Previous[b]	0.358	0.293	0.284	0.343
Complete mixing[c]	0.340	0.284	0.328	0.386
Muon-catalyzed *d-d* fusion				
Present[a]	0.185	0.104	0.175	0.224
Previous[b]	0.192	0.108	0.166	0.215
Complete mixing[c]	0.171	0.097	0.194	0.244

[a] $\sigma_{2S\text{-}2P}=\dfrac{5.5\times10^{-3}}{v^{1.8}}a_0^2$ (present value).

[b] $\sigma_{2S\text{-}2P}=\dfrac{3.7\times10^{-3}}{v^{2}}a_0^2$ (from Ref. 5 using the method of Ref. 7).

[c] $\sigma_{2S\text{-}2P}\rightarrow\infty$ (statistical).

ACKNOWLEDGMENTS

We are grateful to Dr. G.M. Hale for advice on the analytic evaluation of some of the integrals. This work was supported by the U.S. Department of Energy, in large part by the Division of Advanced Energy Projects.

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